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# ON DETECTING OUTLIERS IN MIXED POPULATIONS

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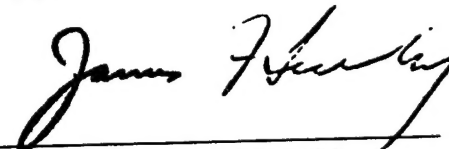**HANSCOM AIR FORCE BASE, MA 01731-3010**


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**13. ABSTRACT (Maximum 200 words)**

In this report we introduce an operational methodology for detecting outliers in data which is a mixture of events from a variety of sources. The only assumption required is that the data contain no previous nuclear events. Thus ground truth data is not required. The method models the data as a mixture of two or more event types. It then develops a test statistic based on a modified likelihood ratio and the bootstrap T. test for outliers. The calculation of this statistic is accomplished by making use of clustering methods to initialize the EM algorithm which is then used to obtain the required maximum likelihood estimates.

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# CONTENTS

# 1. Introduction

Monitoring a comprehensive test ban treaty involves the difficult problem of differentiating the seismic signal of nuclear events from the overwhelming amount of seismic signals from earthquakes, mining explosions, etc. This problem is made even more difficult due to the lack of information concerning the behavior of nuclear signals. Furthermore, in many regions, little information is available on the background events.

Wang, et. al. (1996) frame the problem of detecting nuclear events in terms of detecting outliers (nuclear events) from a mixture population (earthquakes, mining explosions, etc.). The authors develop a modified likelihood ratio test that requires no distributional assumptions concerning the outlier distribution, which is a powerful practical solution to the lack of well established training samples for nuclear events. Using the bootstrap to model the distribution of the test statistic and calculate critical values, the authors show this modified test is as powerful as the standard likelihood test in which complete information concerning the distribution of the outlier population is known. However, the training data used to model the mixture distribution was assumed to be "pure", meaning that information concerning the source of the events in the training data is assumed to be known. A brief summary of the test statistic and the bootstrap procedure is given in Appendix B.

In this report, the problem of detecting the rare seismic signal from events in new or relatively unexplored regions is studied. Extending the work of Wang, et. al. (1996), a two stage procedure is introduced that first examines a potential training sample from a previously unexplored region for potential outliers, readying the training sample for testing new data. Second, additional information is incorporated in an attempt to identify the

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sources of the events in the training sample for research purposes. However, we should stress in this approach introduced here, it is not necessary to be able to label events. The only assumption made regarding the nature of previous events is that none of them are nuclear events.

## 2. The Procedure

In this section, the procedure for screening data about which little information about the source of the events is known, such as data collected from a new region of interest, is developed. The data are assumed to be uncontaminated, i.e. containing no nuclear events, and are known to contain a fixed number of groups. These groups represent the types of non-nuclear seismic activity in a region. Examples include earthquakes and mining blasts. The data can include any number of characteristics calculated from the seismic signals. A flowchart of the procedure is given in Figure 1.

The first step involves clustering the data using the method of hierarchical clustering discussed in Appendix A. After the clustering stage, initial estimates of the parameter values are calculated from the estimated group membership. It is possible that in certain situations, particularly when the groups in the training sample overlap, the clustering algorithm will return one or more clusters that are considerably smaller than is reasonable. In such cases, these small clusters are temporarily set aside, and the remaining data is used to form clusters and estimate initial parameters.

Now, each point is considered individually by the using the other $n - 1$ points as a pseudo training sample. The modified likelihood test developed in Wang, et. al. (1996) is used to test each point and determine the probability that each point belongs to the assumed

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          ┌─────────────────┐
          │     Cluster     │
          │    Analysis     │
          │   (k fixed)     │
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          │    Calculate    │
          │ Starting Values │
          │i.e. Initial Parameter│
          │    Estimates    │
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          ┌─────────────────┐        ┌──────────────┐
          │Test Training Data│──────▶│   OUTLIERS   │
          │      using      │        └──────────────┘
          │  Leave-One-Out  │
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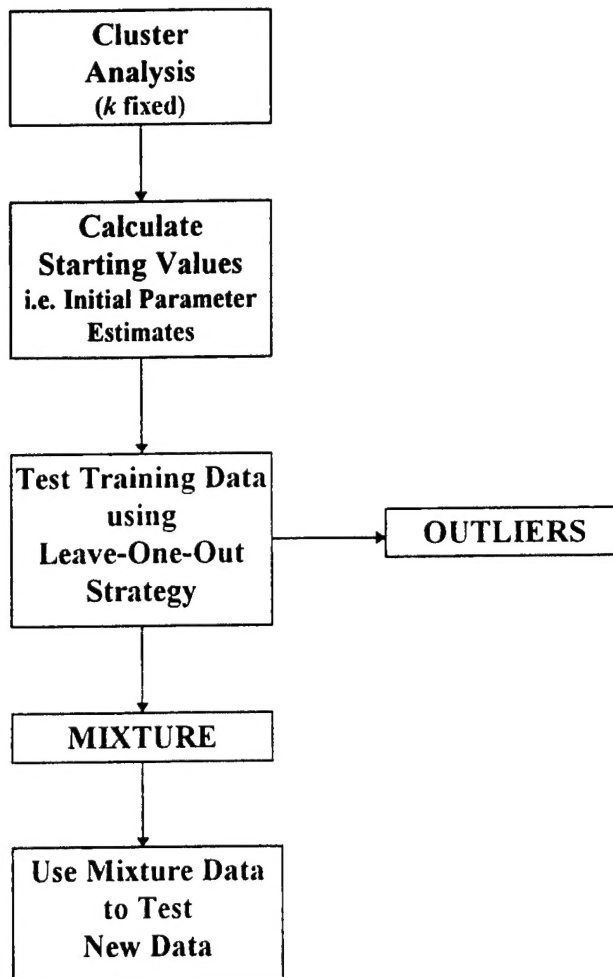
**Figure 1**

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mixture population. Any point with a significant result (probability of inclusion in the mixture is small) at this phase is labeled an outlier and removed from the future training data. The other points tested as belonging to the mixture can now be used as a "clean" training data set for testing inclusion of future events in the mixture.

## 2.1 Example

The data for this example are the result of an analysis of earthquakes and mining explosions from the Vogtland region near the Czech-German border done by Relu Burlacu and Eugene Herrin from the Department of Geological Sciences at the Southern Methodist University. These data were taken from the ground truth database put together by Grant, et. al. (1993). The procedure used to generate the measurements is new to the seismic community and involves fitting a low-order (usually third) autoregressive process to the Lg-phase of the waveform. The power spectral density is estimated and the strength and frequencies of the real and complex poles are calculated. Burlacu and Herrin report that a characteristic pattern appears, namely that distributed surface explosions tend to be lower frequency with a sharper spectrum (strong pole) and that earthquakes tend to have higher frequencies and a more distributed spectrum (weak pole). These features are incorporated into a promising screening process to identify mining blasts. Here, the complex frequency and pole strength are used to demonstrate this new algorithm.

Table 1 contains information on the events used in this study and Figure 2 shows a scatterplot of the complex frequency and pole for each event (plotting characters indicate event number). Note that event number 25 is listed in the ground truth data base as an explosion, although some controversy has surrounded this event. For this example, the ground truth information is not used. Rather, the source for each event is assumed to be

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## Table 1

| Event # | Date | Lat(N) | Long(E) | Depth | $M_l$ | Y (kg) | Or. time | Q/X |
|---|---|---|---|---|---|---|---|---|
| 1 | 031191 | 50.207 | 12.685 | 0 | 1.98 | 3,265 | 12:03:24 | X |
| 2 | 032191 | 50.207 | 12.685 | 0 | 2.05 | 3,982 | 12:04:15 | X |
| 3 | 032291 | 50.207 | 12.685 | 0 | 2.03 | 2,835 | 12:33:25 | X |
| 4 | 032391 | 50.207 | 12.685 | 0 | 1.99 | 2,025 | 12:00:56 | X |
| 5 | 032491 | 50.296 | 12.225 | 12.9 | 2.18 | - | 05:05:04 | Q |
| 6 | 032491 | 50.279 | 12.228 | 12.9 | 1.50 | - | 05:35:21 | Q |
| 7 | 032491 | 50.277 | 12.240 | 13.9 | 1.40 | - | 06:57:59 | Q |
| 8 | 032491 | 50.278 | 12.220 | 12.4 | 1.65 | - | 09:38:33 | Q |
| 9 | 032491 | 50.294 | 12.223 | 12.7 | 2.07 | - | 14:33:28 | Q |
| 10 | 032491 | 50.293 | 12.224 | 12.5 | 1.80 | - | 15:00:45 | Q |
| 11 | 032491 | 50.293 | 12.224 | 9 | 1.73 | - | 15:41:04 | Q |
| 12 | 032591 | 50.298 | 12.222 | 12.9 | 2.37 | - | 14:54:14 | Q |
| 13 | 032591 | 50.292 | 12.213 | 12.4 | 1.54 | - | 22:31:46 | Q |
| 15 | 050291 | 50.207 | 12.713 | 0 | 1.93 | 3,575 | 11:06:10 | X |
| 19 | 051991 | 50.360 | 12.371 | 0 | 2.06 | - | 03:22:10 | Q |
| 20 | 052391 | 50.207 | 12.713 | 0 | 2.12 | 3,135 | 11:01:05 | X |
| 21 | 052591 | 50.207 | 12.713 | 0 | 2.13 | 3,135 | 11:01:29 | X |
| 23 | 052891 | 50.207 | 12.685 | 0 | 2.01 | 3,575 | 11:03:51 | X |
| 24 | 062091 | 50.207 | 12.685 | 0 | 1.98 | 1,998 | 11:01:17 | X |
| 25 | 062091 | 50.293 | 12.803 | 0 | 1.80 | - | 11:45:35 | X |
| 26 | 062291 | 50.207 | 12.685 | 0 | 2.15 | 2,886 | 10:58:34 | X |
| 27 | 062791 | 50.207 | 12.685 | 0 | 1.93 | 3,515 | 11:04:40 | X |
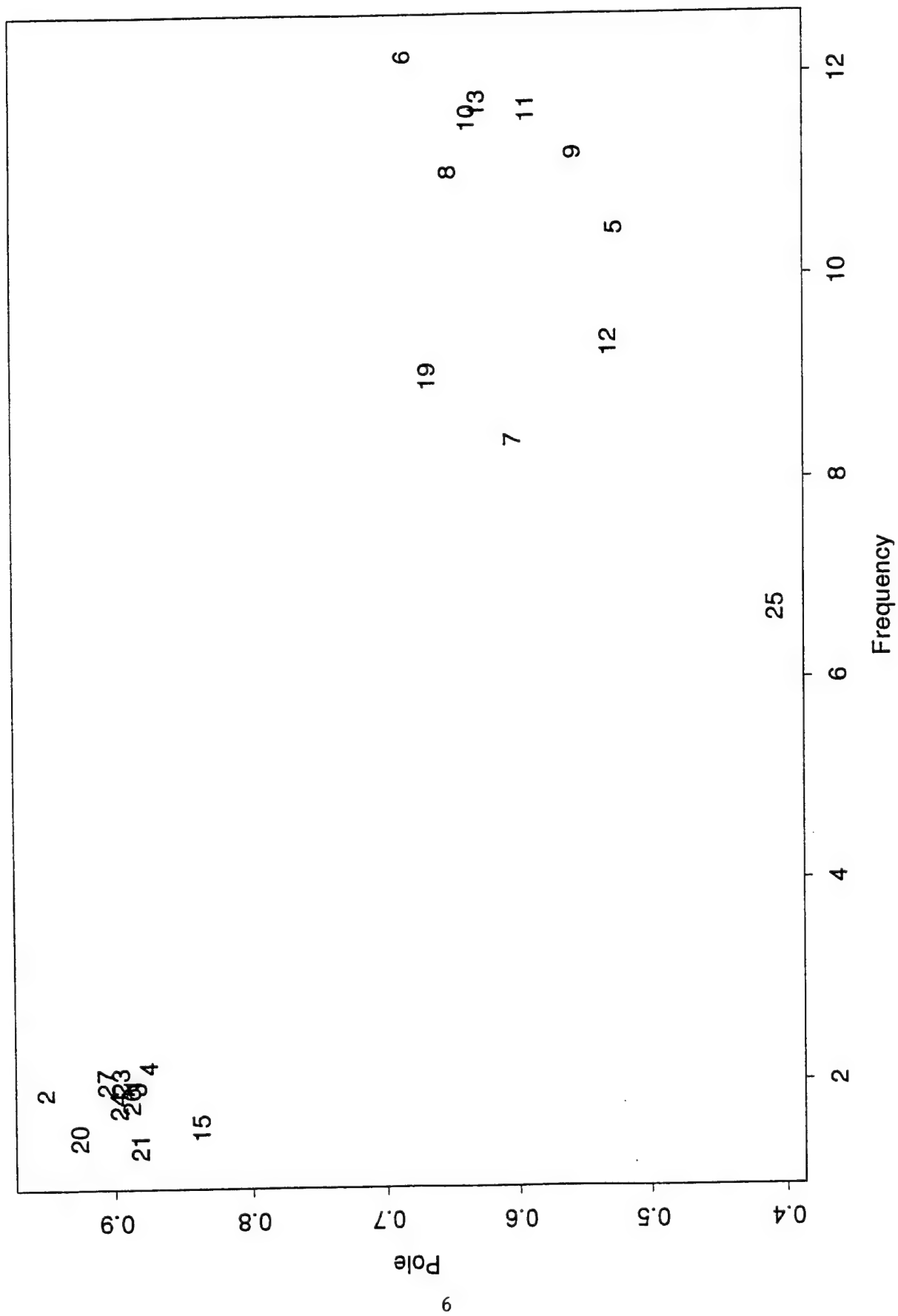
Figure 2: Scatterplot of Frequency vs. Pole

unknown, although it is assumed that the data set is composed of observations from two sources (earthquake and mining blast). Finally, it is also assumed that no nuclear events are present in the sample.

Figure 3 shows the result of the cluster analysis. The members of each cluster are indicated on the plot (as a "1" or a "2") as well as a 95% contour for each component normal distribution using the parameters estimated from the results of the cluster analysis. Note that the labeling of clusters is arbitrary and does not indicate the source of the event. These data show a clear separation between the groups. Hence only one iteration of the cluster analysis is necessary.

Figure 4 shows the results of the leave-one-out testing procedure. Plotted are the p-values for being in the mixture associated with each frequency and pole pair (plotting characters indicate p-value). Note that only event 25 shows a significant result (p-value = 0.01), which leads to the conclusion that event 25 is an outlier to the mixture distribution of earthquakes and explosions. Results for all other points support their membership in the mixture and are consistent with the ground truth information.

New data values in this region could now be tested using this "clean" data. In fact, Figure 5 shows contours representing effective rejection regions ($\alpha$ = 0.1, 0.05, 0.01) based on this training sample. Note that these regions mirror the shape of the distributions suggested by the data.
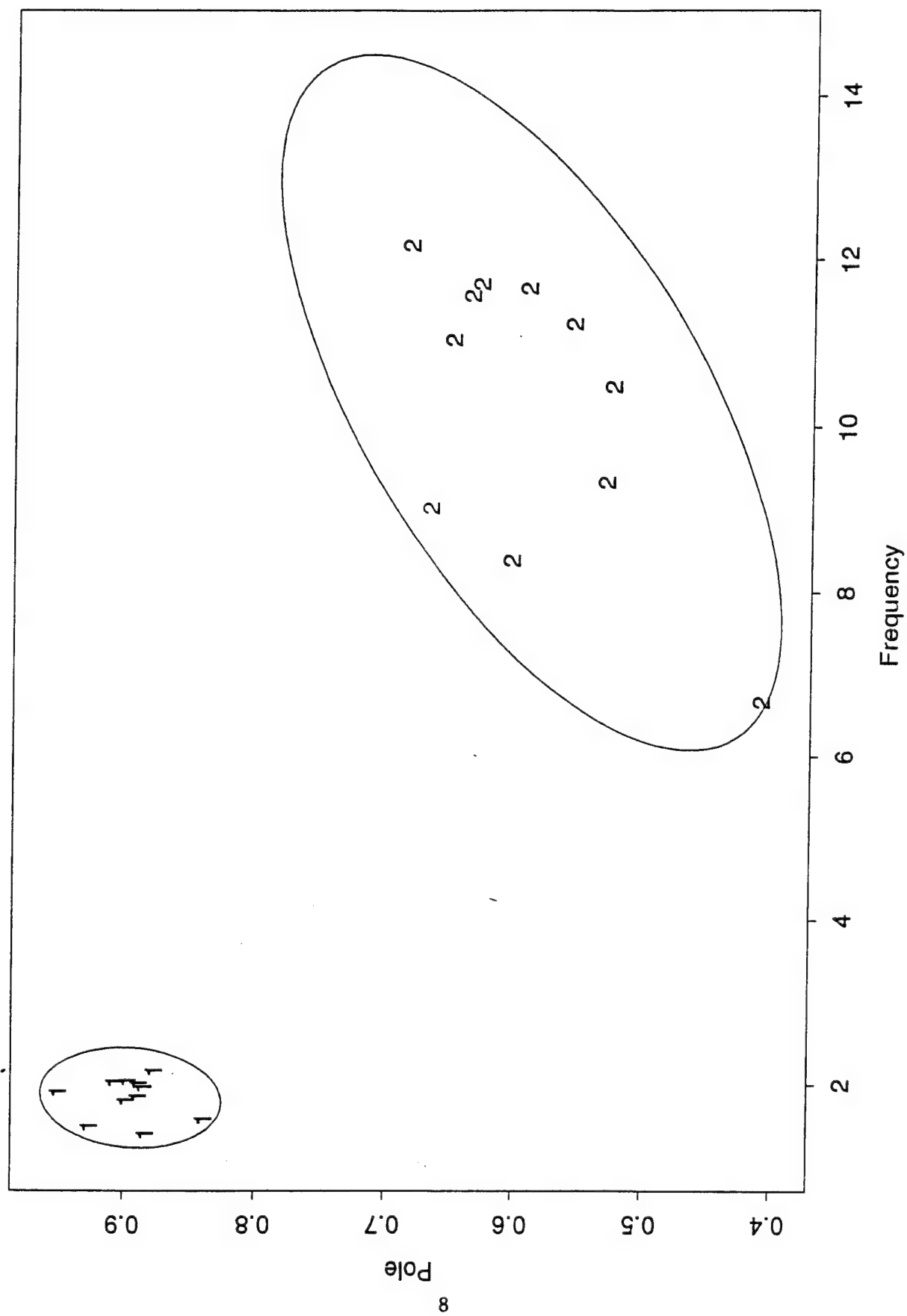
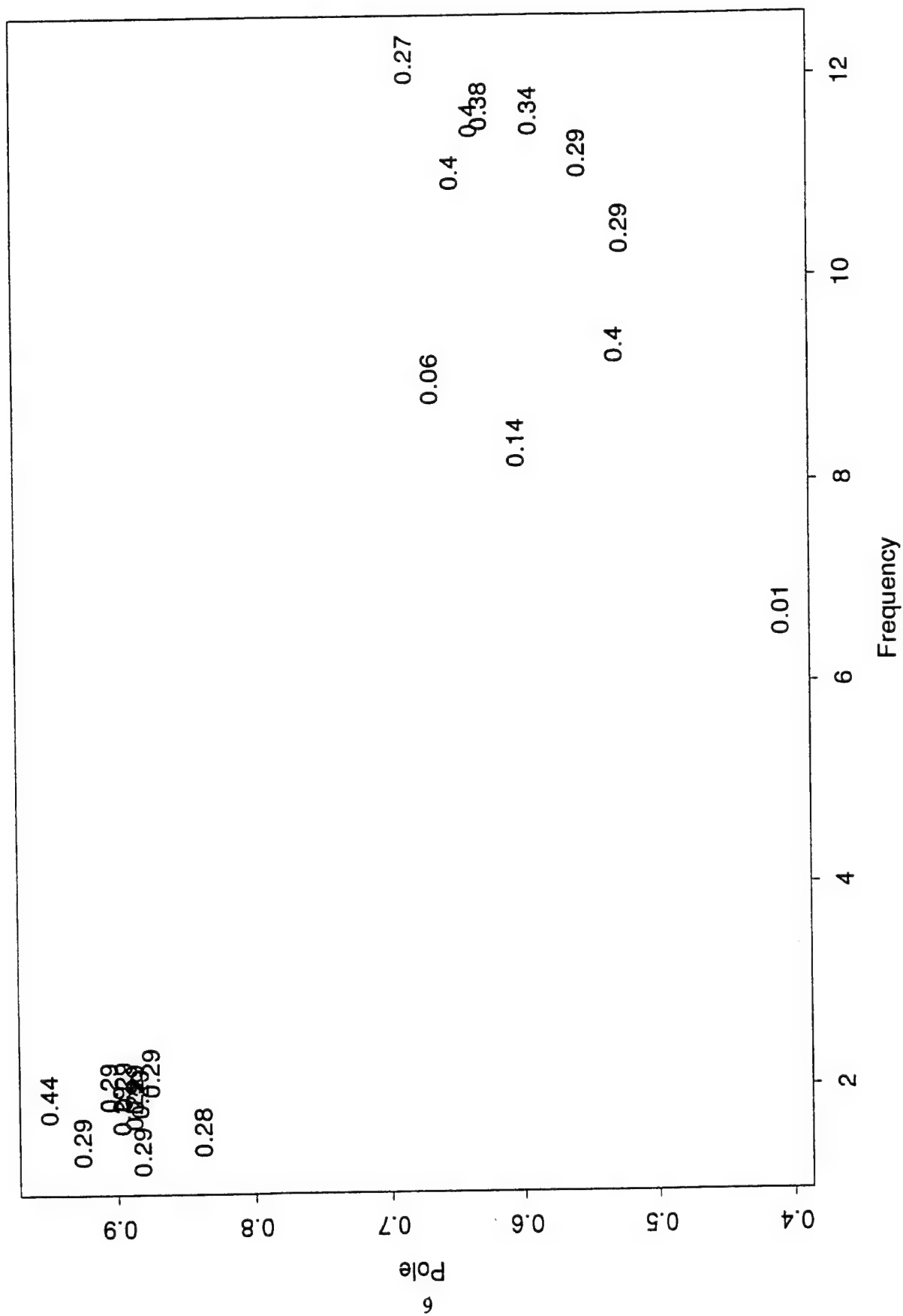Figure 3: Results of Cluster Analysis

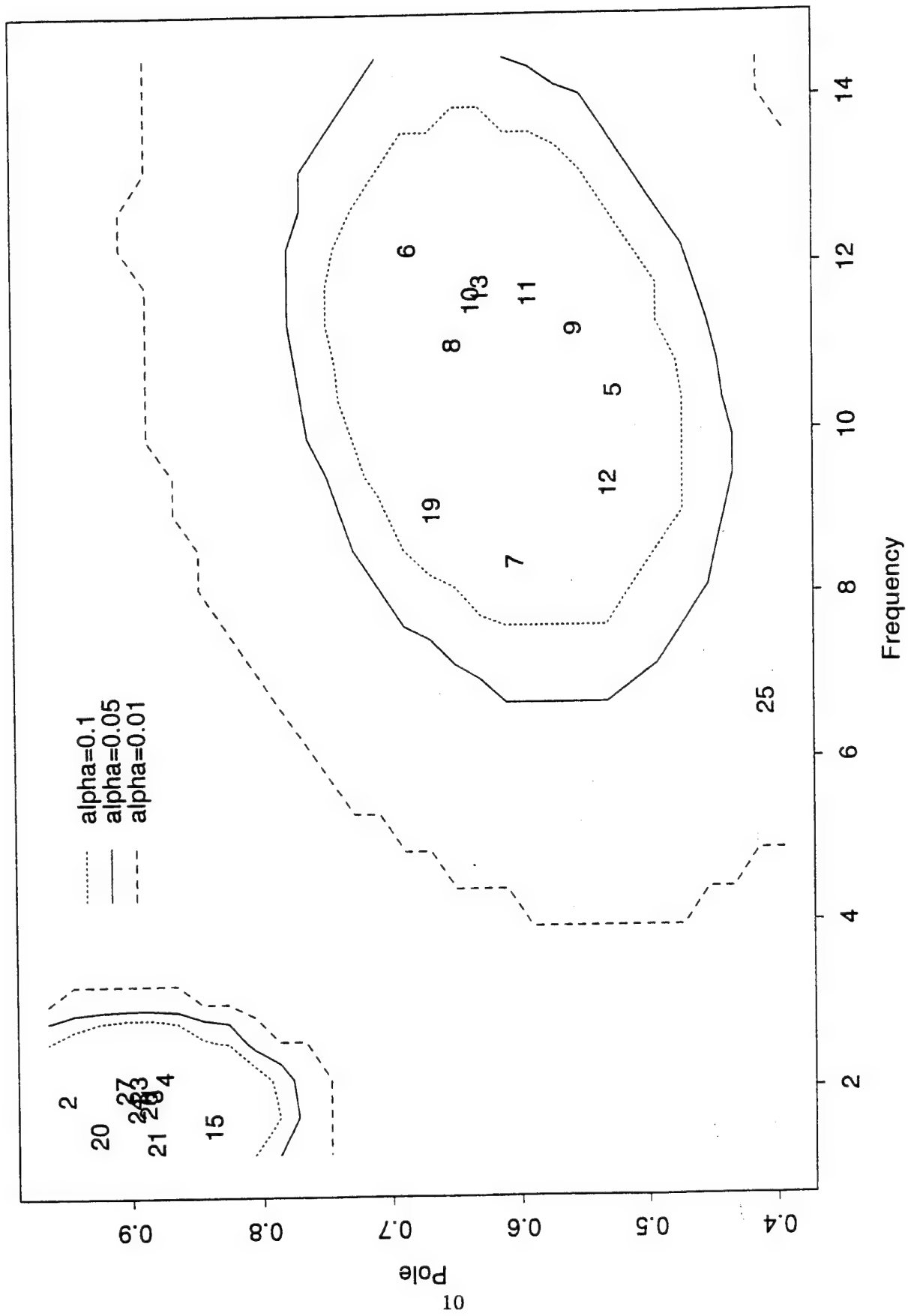Figure 4: Results of Leave-One-Out Analysis

Figure 5: Rejection Regions

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1. Grant, L., Coyne, J., and Ryall, F. (1993), "CSS Ground Truth Database: Version I Handbook," *Scientific Report,* C93-05, Center for Seismic Studies.

2. Seber, G.A.F. (1984), *Multivariate Observations,* John Wiley & Sons, New York.

3. Wang, Woodward, Gray, Wiechecki and Sain (1996), "A New Test for Outlier Detection from a Multivariate Mixture Distribution," submitted to *Journal of Computational and Graphical Statistics*.

## Appendix A: Hierarchical Clustering

Clustering is the process of grouping similar objects on the basis of characteristics of the objects. The process is also referred to as classification or pattern recognition. For a general treatment of the subject, see, for example, Seber (1984) or any textbook on multivariate statistics.

Two basic types of clustering algorithms exist. The first is hierarchical clustering, which is an iterative technique involving the grouping of smaller clusters into larger ones until the desired number of clusters has been achieved. The second type partitions objects into non-overlapping groups by setting the number of clusters, choosing initial locations of the clusters, and then assigning points to one of the groups according to some pre-specified criterion. In this work, a two-stage approach to clustering is taken. First, a hierarchial approach is used to obtain initial parameter estimates of the clustering. Then, in some cases, a procedure similar in nature to the $k$-means approach of Hartigan (1975) is used to refine the parameter estimates if necessary.

The clustering algorithm begins by considering each of the $n$ data points as an individual cluster. Then, the two points nearest to each other are combined to form $n - 1$ clusters. The procedure continues by combining or fusing the two clusters that are the most similar at each iteration. Here, similarity is a distance measure that is calculated in a variety of ways. The three most common measures of similarity are single linkage (nearest neighbor), complete linkage (farthest neighbor), or the nearest centroid measure. For single linkage, the similarity between two clusters is measured as the smallest distance between a point of one cluster and a point of another. On the other hand, complete linkage measures similarity between two clusters as the largest distance between a point of one cluster and a

point of another. The centroid method measures similarity as the distance between the centroids or means of the points in each cluster.

Both the single and complete linkages suffer from the extreme nature of the measure of similarity. Single linkage causes clusters formed by a single individual to be more likely to join another established cluster rather than forming the nucleus of a new cluster. This phenomenon, known as "chaining," leads to clusters that are formed of smaller groups linked together by intermediates. Complete linkage yields the opposite effect as individuals are more likely to form a new cluster than join established ones. This has the potential to yield clusters that are formed of points that do not really belong together. The centroid method is more robust than either of these two measures and is less subject to these problems in the formation of clusters. Hence, the centroid method is the measure adopted in this work.

**Appendix B**

# A New Test for Outlier Detection from a Multivariate Mixture Distribution

Suojin Wang, Wayne A. Woodward, H.L. Gray, Stephen Wiechecki, and Stephan Sain

## ABSTRACT

The problem of testing an outlier from a multivariate mixture distribution of several populations has many important applications in practice. One particular example is in monitoring worldwide nuclear testing, where we wish to detect whether an observed event is possibly a nuclear explosion (an outlier) by comparing it with the training samples from mining blasts and earthquakes. The combined population of seismic events from mining blasts and earthquakes can be viewed as a mixture of two populations. The classical likelihood ratio test appears to be not applicable to our problem, and in spite of the importance of this problem, little progress has been made in the literature. In this report we propose a simple modified likelihood ratio test that overcomes the difficulties in the current problem. Bootstrap techniques are used to approximate the distribution of the test statistic. The advantages of the new test are demonstrated via simulation studies. Some new computational findings are also reported.

# 1. Introduction

An extremely important practical problem is that of monitoring worldwide nuclear testing, where we wish to detect whether an observed seismic event may be a nuclear explosion by comparing it with the training samples obtained from previous seismic activity in the region. In this case, the training data will often be composed of data which are a composite of mining explosions and earthquakes. Usual methods of outlier detection typically focus on the setting in which observations are tested as outliers from a single population. However, in the case considered here, there are two populations, and we wish to test whether a seismic event should be considered to be an outlier from either or both of the populations. Actually, these results are applicable to two or more populations but we focus on the case of two. Another point of interest is the fact that the setting considered here differs from a common outlier scenario in which a sample is given and the observations from the sample are tested to determine whether they should be considered as outliers from the population from which the sample was obtained. This, however, is not the scenario considered here. Specifically, in our setting, "pure" samples from the populations in question are available, and our desire is to test a new observation as an outlier from these populations. We will refer to this testing procedure as outlier testing throughout the report.

The classical method for outlier detection of the type we are addressing is the likelihood ratio test (Wilks (1963), Caroni and Prescott (1992)), usually under the normality assumption for the multivariate distributions of the training sample population and the outlier population, and under the assumption of equal covariance of the two populations under the alternative hypothesis. The resulting test is essentially the Hotelling's $T^2$ test (see Anderson (1984)). In our current problem, because of the fact that there is not a single multivariate normal population associated with the training sample, these assumptions are not satisfied. Thus, a direct application of the standard likelihood ratio test does not seem possible. In spite of the importance of this problem, to our knowledge little progress has been made in the literature. Baek et al. (1992) recently considered the outlier testing in the seismic setting discussed here but in the special case in which seismic events are tested as outliers from a single population, usually earthquakes. Baek et al.

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(1992) used a bootstrap approach to ascertain the distribution of the likelihood ratio when the multivariate distribution associated with the training sample has both continuous components and discrete components that have a finite number of possible outcomes. Some assumptions, such as equality of covariances, are imposed to link the training sample population and the outlier population. It is possible to apply the test of Baek et al. sequentially to each training sample population, but this can be cumbersome, e.g. the training sample populations often have different covariance structures. Furthermore, this procedure would result in substantial loss of power.

In this report we consider an approach to the practical problem at hand by considering the combined population of seismic events of mining blasts and earthquakes as a mixture of two populations. We propose a simple modified likelihood ratio test using bootstrap resampling that appears to perform well in this setting. The methodology is presented in Section 2 for testing outliers from a mixture population consisting of $m$ components. Some numerical procedures are addressed, including the use of the bootstrap for approximating the distribution of the test statistic in Section 3. We also describe how the intensive computing time required for the bootstrap resampling can be reduced without loss of accuracy when the training sample size is relatively large. Section 4 provides the results of empirical studies. Some concluding remarks are given in Section 5.

## 2. The Methodology

Suppose we have a mixture distribution $\Pi$ of $m$ populations, $\Pi_i$, $i = 1, ..., m$. In the nuclear testing example mentioned above, $m = 2$ for mining explosions and earthquakes. Let $d$ be the dimension of the variables from the mixed population $\Pi$, and for clarity in the presentation assume all the distributions are continuous. Note that extensions to discrete or mixed cases are mainly a matter of notational adjustments. The density of the mixture distribution is

$$f(\boldsymbol{x}; \boldsymbol{\theta}) = \sum_{i=1}^{m} p_i g_i\left(\boldsymbol{x}; \theta_i\right),$$

(1)

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where $p_i \geq 0$ are mixing proportions with $\sum_{i=1}^{m} p_i = 1$, $g_i$ are the densities of $\Pi_i$, $\theta_i$ are unknown parameter vectors, $\boldsymbol{\theta} = (p_1, ..., p_m, \theta'_1, ..., \theta'_m)'$ and $\boldsymbol{x} = (x_1, ..., x_d)'$. In the nuclear monitoring scenario, we wish to test whether a new seismic event is an outlier to the mixture of earthquakes and mining explosions. More generally, we wish to be able to test whether a new observation is an outlier from the mixed population $\Pi$.

Assume that we have a random training sample of size $n$ from the mixture population

$$X_1, ..., X_n \in \Pi,$$

and that we are able to identify the associated source population for $n_L \leq n$ members of the training sample. For convenience, let

$$X_{k_{i-1}+1}, X_{k_{i-1}+2}, ..., X_{k_i} \in \Pi_i, \text{ for } i = 1, ..., m, \tag{2}$$

where $0 = k_0 < k_1 < ... < k_m = n_L$, i.e., $n_i = k_i - k_{i-1}$ (normally $\geq 10$) data points are identified to be from $\Pi_i$. Additionally, we allow for the possibility that the training sample contains $n_U$ unlabeled observations from the mixture. In the notation of Redner and Walker (1984) we assume the sample $X_1, ..., X_n$ is of Type 4, i.e. the training sample consists of labeled and unlabeled observations. The associated $n_i$'s, $i = 1, ..., m$ are random variables following a multinomial distribution, and they contain information about the mixing proportions. In this notation, $n = n_L + n_U$. If in fact $n_U = 0$, then the training sample consists of only labeled observations and is a sample of Type 3 using the Redner and Walker notation. Now a new observation $X_{n+1}$ is obtained. Given (2) we want to test the following hypotheses:

$$H_0 : X_{n+1} \in \Pi$$

vs. $\tag{3}$

$$H_1 : X_{n+1} \notin \Pi.$$

The classical likelihood ratio test statistic is the ratio of the maximized likelihood functions under $H_0$ and $H_1$. Under $H_0$ the sample is of Redner and Walker Type 4, i.e. we assume that

$X_1, ..., X_n$ are as before while $X_{n+1}$ is unlabeled but from the same mixture distribution as $X_1, ..., X_n$. That is, we assume that all $n + 1$ observations are from the mixture distribution assumed under $H_0$ with $n_L$ of these labeled and $n_U + 1$ unlabeled. The likelihood function under $H_0$ is

$$L_0(\theta) = \frac{n_L!}{n_1! \ldots n_m!} \left( \prod_{i=1}^{m} \prod_{j=k_{i-1}+1}^{k_i} p_i g_i(X_j; \theta_i) \right) \left( \prod_{s=n_L+1}^{n} f(X_s; \theta) \right) f(X_{n+1}; \theta).$$

Let $h(x; \alpha)$ be the density associated with the outlier population from which $X_{n+1}$ is sampled, where $\alpha$ is an unknown parameter vector. Then the likelihood function under $H_1$ is

$$L_1(\theta, \alpha) = \frac{n_L!}{n_1! \ldots n_m!} \left( \prod_{i=1}^{m} \prod_{j=k_{i-1}+1}^{k_i} p_i g_i(X_j; \theta_i) \right) \left( \prod_{s=n_L+1}^{n} f(X_s; \theta) \right) h(X_{n+1}; \alpha). \qquad (4)$$

Difficulties arise when maximizing $L_1$ since there is only a single observation from the outlier population so that generally no suitable MLE is possible for $\alpha$, unless $\alpha$ is assumed to directly link to $\theta$. Any such linkage assumption is quite questionable since we now have $m$ individual populations that make up the mixture distribution. Furthermore, with only one observation it is impossible to do any model checking of $h(x; \alpha)$. To overcome these difficulties and to observe the fact that little information is known about the outlier population from which $X_j$ is sampled, we simply use a constant density $h(x) \equiv c$ over its practical (finite) support. Moreover, the constant density is also assumed in the bootstrap procedure described below. Thus, dropping the constant from the likelihood ratio test statistic will not affect any test conclusions. Therefore we let

$$\widetilde{L}_1(\theta) = \frac{n_L!}{n_1! \ldots n_m!} \left( \prod_{i=1}^{m} \prod_{j=k_{i-1}+1}^{k_i} p_i g_i(X_j; \theta_i) \right) \left( \prod_{s=n_L+1}^{n} f(X_s; \theta) \right),$$

which is the likelihood based on the sample $X_1, ..., X_n$ from the mixture. We define a simple modified likelihood ratio test statistic

$$W = \frac{\sup\limits_{\theta \in \Theta} L_0(\theta)}{\sup\limits_{\theta \in \Theta} \widetilde{L}_1(\theta)}, \tag{5}$$

where $\Theta$ is the entire parameter space. It is easily seen that the departure of $X_{n+1}$ from $f$ will reduce $\sup\limits_{\theta \in \Theta} L_0(\theta)$ making $W$ small. Hence the rejection region is of the form $W \leq W_\alpha$ for some $W_\alpha$ picked to provide a level $\alpha$ test. Since the null distribution of $W$ has no known closed form, we suggest the use of the parametric bootstrap method to approximate it, as shown in the next section. Based on the discussion here the use of $W$ seems to be a reasonable approach, and in Section 4 we demonstrate that $W$ performs well under all the simulation scenarios considered.

Concluding this section, we point out that asymptotically $W \approx f(X_{n+1}; \widehat{\theta}_n)$, as $n \to \infty$, where $\widehat{\theta}_n$ is the MLE using the training sample only. See the Appendix for the proof. Moreover, the bootstrap-one method described in the next section is essentially equivalent to using this asymptotic result.

## 3. The Bootstrap and Other Computational Procedures

In this section we discuss numerical issues associated with the test procedure described in Section 3. It should be noted that often both the numerator and denominator of $W$ in (5) may be difficult to obtain since the individual densities are mixture distributions. Recall also that for the numerator we assume that $X_1, \ldots, X_n$ can be identified with their component population, but $X_{n+1}$ is only known to be from the mixture, not the exact component. However, if we consider the setting of multivariate normality for each component, i.e.,

$$g_i(\boldsymbol{x}; \theta_i) \sim N(u_i, \Sigma_i), \tag{6}$$

and thus $f(\boldsymbol{x}; \theta)$ is a mixture of $m$ multivariate normal distributions, a numerical iteration algorithm based on the EM algorithm has been developed by Redner and Walker (1984), for maximizing $L_0(\theta)$. They extended Hosmer's (1973) algorithm for the case of two univariate normal components to the multivariate normal components setting, and in our simulation studies, we have adapted their method. Note that with (6), $\sup\limits_{\theta \in \Theta} \widetilde{L}_1(\theta)$ is easily obtained. Using the

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resulting estimator $\widehat{\theta}_n$ as an initial value in the numerator, it only takes at most a few steps to obtain convergence.

We now turn to bootstrapping the null distribution of $W$. We will employ the parametric bootstrap based on the training sample $X_1, ..., X_n$. The following algorithm is used which mimics the original sampling plan.

**Step 1**: Use (2) to obtain $(\widehat{p}_i, \widehat{u}_i, \widehat{\Sigma}_i)$ for $i = 1, ..., m$.

**Step 2**: For each integer $b$, $b = 1, ..., B$, draw a sample of size $n_L$ from the multinomial distribution with $\widehat{p} = (\widehat{p}_1, ..., \widehat{p}_m)'$. We observe the frequencies $n_{1L}^b$, $n_{2L}^b$, ..., and $n_{mL}^b$ where $n_{1L}^b + n_{2L}^b + \cdots + n_{mL}^b = n_L$. Additionally, we draw a sample of size $n_U$ from the same multinomial distribution resulting in frequencies $n_{1U}^b$, $n_{2U}^b$, ..., and $n_{mU}^b$ where $n_{1U}^b + n_{2U}^b + \cdots + n_{mU}^b = n_U$.

**Step 3**: Draw samples of size $n_{iL}^b$ and $n_{iU}^b$ from $N(\widehat{u}_i, \widehat{\Sigma}_i)$ for $i = 1, ..., m$. The $n_L$ observations associated with frequencies $n_{iL}^b$, $i = 1, ..., m$ are treated as labeled samples in the analysis, while the $n_U$ observations corresponding to $n_{iU}^b$, $i = 1, ..., m$ are treated as unlabeled observations. These resampled data are used to compute the test statistic in (5). This test statistic is denoted by $W_b^*$.

**Step 4**: Draw a new, $(n+1)$st, observation from the empirical mixture by randomly selecting a single observation from the multinomial distribution in Step 2. This multinomial will essentially select a component $i$ between 1 and $m$, and we generate an observation from the associated $N(\widehat{u}_i, \widehat{\Sigma}_i)$ distribution.

**Step 5**: Repeat Steps 2 to 4 $B$ times ($b = 1, ..., B$). Then define $W_\alpha$ to be the $(100\alpha)$th percentile of all $W_b^*$. Specifically, if $\alpha = j/(B+1)$, then $W_\alpha$ is the $j$th smallest value of $\{W_b^*\}_{b=1}^B$ (see McLachlan, 1987). Statistical decisions can then be made.

Notice that when $n$ is large the bootstrap scheme may require considerable computing time. However, when $n_i$ are not very small, this computational burden can be avoided by employing an approximate bootstrap scheme, called bootstrap-one. This technique uses the original training sample in Steps 2 and 3 for all $b = 1, ..., B$. It effectively eliminates these two steps and many calculations in obtaining $W_\alpha$.

The bootstrap-one method conceptually approximates the conditional distribution of $W$ given $X_1, ..., X_n$. When all $n_i$ are relatively large, the conditioning effect is minimal. The accuracy and advantages of the bootstrap-one method are among the things studied in simulations which are discussed in the next section.

## 4. Empirical Studies

In this section we report some results of a simulation study to illustrate the performances of the new methods. In these simulations we focus on the case in which all training sample observations are labeled, i.e. $n_U = 0$.

**Example 1.** In this example, we choose $m = 1$, $d = 2$, and $n = 40$ so that the training sample is from a bivariate $N(\mu, \Sigma)$, where

$$\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \qquad \Sigma = \begin{pmatrix} 1 & .5 \\ .5 & 1 \end{pmatrix} \tag{7}$$

were used. Obviously, in this case since there is only one component in the "mixture", all observations in the training sample can be labeled, i.e. $n_U = 0$. The reason for choosing $m = 1$ is that in this case it is easy to apply the standard likelihood ratio test assuming that the outlier population is normal with the same covariance $\Sigma$. In this case, there is a single training sample of size $n$ and an observation $X_{n+1}$ to be tested as an outlier. Baek et al. (1992) discusses the generalized likelihood ratio test in this setting. In particular, the likelihood ratio statistic is given by

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$$\lambda = \frac{\sup_{\theta \in \Theta} L_0(\theta)}{\sup_{\theta \in \Theta} L_1(\theta, \alpha)} \; , \tag{8}$$

where $L_1(\theta, \alpha)$ is given in (4) and $\alpha$ is related to $\theta$ in a certain way.

Specifically, $h$ is the multivariate normal density associated with observation $X_{n+1}$ and $\alpha = (\mu_2, \Sigma)$ is estimated by taking $\hat{\mu}_2 = X_{n+1}$ and taking $\hat{\Sigma}$ to be the MLE obtained from the training sample. Under the normality assumption in this example, the test statistic in (8) is known to be distributed as Hotelling's $T^2$ (e.g. Anderson, 1984). Baek et al. (1992) considered the likelihood ratio in (8), where the multivariate random variables could be composed of both continuous and discrete components. They approximated the distribution of $\lambda$ in this case using the bootstrap procedure described here. They applied the bootstrap procedure to the special case in which the distributions were multivariate normal and approximated the distribution of $\lambda$ using the bootstrap procedure. Simulations have shown that the power of the test based on the bootstrap is very similar to that obtained based on Hotelling's $T^2$ in the multivariate normal case. In this report all tests are based on the use of bootstrap resampling to approximate the distribution of the test statistic. The test based on (8) will be called the "standard" likelihood ratio test.

Instead of including $L_1(\theta, \alpha)$ in the denominator of (8) in this multivariate normal setting, we could have used the test statistic given in (5) which is based on the use of a constant density $h(x) = c$ for over its support. The test statistic using (5) will be termed the "modified" likelihood ratio test. For each of these tests, whenever we approximate the distribution of the test statistic by a full bootstrapping of $n+1$ observations, we will refer to this as the "full" procedure. Alternatively, in each case we also consider the use of the bootstrap-one technique. In Table 1 we denote them as "full" and "one" respectively.

Table 1 summarizes the simulation results of the two tests. One thousand replications were used for each entry and we used $B = 499$. The power was obtained with $N\left(\binom{2}{2},\right.$

$$\begin{pmatrix} 1 & -.5 \\ -.5 & 1 \end{pmatrix} \Bigg)$$ as the outlier population. We have experimented with other covariance values, including that in (7), and similar power patterns were observed.

First, we compare the standard and modified tests using full bootstrapping. In Table 1, it can be seen that the significance levels for both tests are close to the nominal level of $\alpha = .05$ with the modified tests having slightly larger levels. Additionally, the powers of the two tests are similar with the modified tests having somewhat larger power. Thus, the use of $W$ in (5), which appropriately reflects our ignorance about the outlier population, performs as well as the full likelihood ratio.

Next, comparing "One" columns to "Full" columns, we observe that the bootstrap-one has significance levels that are artificially high for smaller sample sizes. However, for large $n$ (say $\geq$ 100) the significance levels are of appropriate size. For these larger sample sizes the bootstrap-one procedure tended to have higher power than obtained using full bootstrapping. Based on these results and the computational burden associated with large $n$ suggests that the bootstrap-one is a viable alternative. Finally, notice that the bootstrap-one method is identical for the standard and new tests. In fact, the identity can be shown analytically under normality. However, the identity is not true in general.

Example 2. In this example we consider the use of the likelihood ratio test to test for outliers from the mixture model in (1) with $m = 2$ and $n = 60$. Again we consider the case in which $d = 2$ and $n_U = 0$, and specifically, we assume that the component densities $g_1$ and $g_2$ are multivariate normal densities associated with a

$$N\left( \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & .5 \\ .5 & 1 \end{pmatrix} \right)$$

and

$$N\left( \begin{pmatrix} 2 \\ 2 \end{pmatrix}, \begin{pmatrix} 1 & -.5 \\ -.5 & 1 \end{pmatrix} \right)$$

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populations respectively.

*Case a:* $p_1 = p_2 = .5$.

We examine the power of the test for detecting outliers from

$$N\left(\begin{pmatrix} 1+k-5 \\ 1-(k-5) \end{pmatrix}, \begin{pmatrix} 1 & .5 \\ .5 & 1 \end{pmatrix}\right)$$

population where $k = 1, ..., 9$. In Figure 1(a) we show data from a mixture of two populations with $p_1 = p_2 = 0.5$ along with 5 outliers. In Figure 1(b) we show the same data with individual observations labeled with regard to the associated component population or outlier population. The outliers are indicated by solid dots. In Figure 1(c) we again show the labeled data along with contours of the mixture population. Finally, in Figure 1(d) we show means and contours of the two component populations and of the outlier population. In Figure 2 we show the contours of the mixture components as in Figure 1(d) along with the outlier means $(1+k-5, 1-(k-5))'$, $k = 1, ..., 9$. Also in this figure we show the contour of the outlier population for the case $k = 2$, i.e. the mean is $(-2, 4)'$. In Table 2(a) $n = 60$ is used and the nominal level is $\alpha = 0.05$. As can be seen, the significance level is close to the nominal level. Whenever the outlier population is well separated from the component distributions of the mixture we have good power while as would be expected the power lowers dramatically for $k$ near 5. The true powers for $k = 1, 2, 3,$ and 4 are the same as those for $k = 9, 8, 7$ and 6 respectively, due to symmetry. The empirical results appear to verify this fact.

*Case b:* $p_1 = 0.25$ and $p_2 = 0.75$.

In this case we consider the same scenario as Case $a$ but with $p_1 = 0.25$ and $p_2 = 0.75$. In Figure 3 we show the plots corresponding to Figure 1 for the case in which $p_1 = 0.25$ and $p_2 = 0.75$, and in Table 2(b) we show results corresponding to those in Table 2(a) for this case. Again, we see that the significance levels are accurate and that powers are similar to those in Table 2(a). It should be noted that due to smaller $p_1$ here, there was a very small fraction

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( < 0.2%) of all bootstrap simulation replications that did not converge with our current program. This problem seems to become more serious when smaller values of $n$ are used. In our analysis we simply skip any bootstrap realization for which convergence was not obtained and generate another one. Another possible approach would be to use the starting values as final estimates for these bootstrap replications.

## 5. Concluding Remarks

In this report we have proposed a simple modified likelihood ratio test for multivariate outlier detections. This new test is not only good for use in general outlier detection problems, but especially applicable when the training sample population is a mixture of several populations. In the new test no assumption is necessary for the covariance structure or any other moments of the outlier population, and in fact no parametric modeling is required for the outlier population. Furthermore, although with weaker assumptions it is more powerful than the standard likelihood ratio test in the simpler non mixture situation in which the standard test applies.

We have also investigated bootstrapping the distributions of the test statistics. The computationally intensive resampling method seems to be quite effective. When the training sample size is large, we have also suggested the bootstrap-one method, which significantly reduces the computing time and seems to have somewhat more power.

It should be noted that the procedure could be extended to cover the case in which all of the training sample observations are unlabeled. This, however, will require dealing with issues such as the use of appropriate starting values and is not considered here.

# APPENDIX

In this appendix, we show that $W \approx f(X_{n+1}; \widehat{\theta}_n)$, as $n \to \infty$, where $W$ is given in (5). Let

$$\widetilde{\ell}_1(\theta) = \ln\{\widetilde{L}_1(\theta)\},$$

$$\ell_0(\theta) = \ln\{L_0(\theta)\} = \widetilde{\ell}_1(\theta) + \ln\{f(X_{n+1}; \theta)\}. \tag{A1}$$

Suppose $\widehat{\theta}_n$ and $\widehat{\theta}_{n+1}$ satisfy the conditions that $\widetilde{L}_1(\widehat{\theta}_n) = \sup_{\theta \in \Theta} \widetilde{L}_1(\theta)$ and $L_0(\widehat{\theta}_{n+1}) = \sup_{\theta \in \Theta} L_0(\theta)$, respectively. Then $\ell_0'(\widehat{\theta}_{n+1}) = 0$ and $\widetilde{\ell}_1'(\widehat{\theta}_n) = 0$. Thus, from

$$
\begin{aligned}
\ell_0'(\widehat{\theta}_{n+1}) &= \ell_0'(\widehat{\theta}_n) + \ell_0''(\widehat{\theta}_n)(\widehat{\theta}_{n-1} - \widehat{\theta}_n) + \text{smaller terms} \\
&= \frac{\partial}{\partial \theta}[\ln\{f(X_{n+1}; \theta)\}]\Big|_{\theta = \widehat{\theta}_n} + \ell_0''(\widehat{\theta}_n)(\widehat{\theta}_{n+1} - \widehat{\theta}_n) + \text{smaller terms},
\end{aligned}
$$

we have

$$\widehat{\theta}_{n+1} - \widehat{\theta}_n = O_p(\tfrac{1}{n}), \tag{A2}$$

since $\ell_0'(\widehat{\theta}_{n+1}) = 0$, $\ell_0''(\widehat{\theta}_n)$ is of order $O_p(n)$, and $\frac{\partial}{\partial \theta}[\ln\{f(X_{n+1}; \theta)\}]\Big|_{\theta = \widehat{\theta}_n}$ is $O_p(1)$. Now by (A1) and (A2),

$$
\begin{aligned}
W &= \exp\{\ell_0(\widehat{\theta}_{n+1}) - \widetilde{\ell}_1(\widehat{\theta}_n)\} \\
&= \exp\{\ell_0(\widehat{\theta}_n) + \ell_0'(\widehat{\theta}_n)(\widehat{\theta}_{n+1} - \widehat{\theta}_n) + O_p(\tfrac{1}{n}) - \widetilde{\ell}_1(\widehat{\theta}_n)\} \\
&= \exp[\ln\{f(X_{n+1}; \widehat{\theta}_n)\}] + O_p(\tfrac{1}{n}) \\
&= f(X_{n+1}; \widehat{\theta}_n) + O_p(\tfrac{1}{n}),
\end{aligned}
$$

completing the proof.

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**Table 1.** Comparisons of significant level and power of the standard likelihood ratio test and modified likelihood ratio test, using two (Full and One) bootstrap approximations.

| $n$ | Significance Level | | | | Power | | | |
|---|---|---|---|---|---|---|---|---|
| | Standard | | Modified | | Standard | | Modified | |
| | Full | One | Full | One | Full | One | Full | One |
| 15 | .048 | .118 | .065 | .118 | .522 | .729 | .568 | .729 |
| 20 | .048 | .100 | .063 | .100 | .541 | .709 | .588 | .709 |
| 25 | .036 | .081 | .048 | .081 | .563 | .704 | .601 | .704 |
| 30 | .047 | .084 | .051 | .084 | .579 | .718 | .609 | .718 |
| 50 | .046 | .064 | .050 | .064 | .626 | .696 | .645 | .696 |
| 100 | .056 | .059 | .057 | .059 | .646 | .677 | .657 | .677 |
| 150 | .059 | .057 | .061 | .057 | .655 | .703 | .665 | .703 |
| s.e. | .007 | | | | .015 | | | |

**Table 2a.** Significance level and power of new test in Example 2; $p_1 = p_2 = 0.5$, $n = 60$, $B = 199$, 1000 replications

| Level | .050 (s.e. .007) | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| $k$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
| Power | 1.000 | .984 | .754 | .226 | .031 | .231 | .767 | .980 | 1.000 |
| s.e. | .001 | .004 | .014 | .013 | .006 | .013 | .014 | .004 | .001 |

**Table 2b.** Significance level and power of new test in Example 2; $p_1 = 0.25$, $p_2 = 0.75$, $n = 60$, $B = 199$, 1000 replications

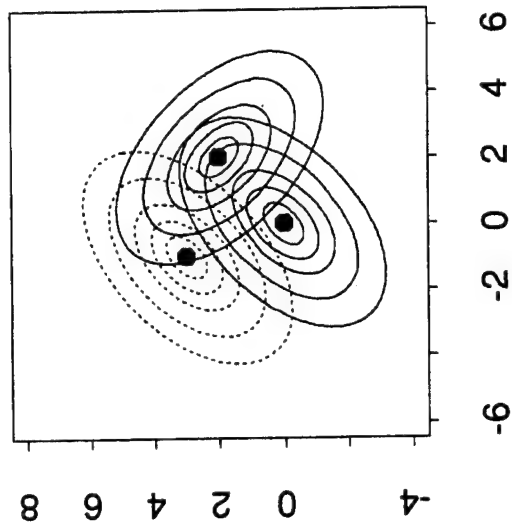| Level | .055 (s.e. .007) | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| $k$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
| Power | .999 | .970 | .709 | .245 | .042 | .242 | .701 | .972 | .999 |
| s.e. | .001 | .005 | .014 | .014 | .006 | .014 | .014 | .005 | .001 |
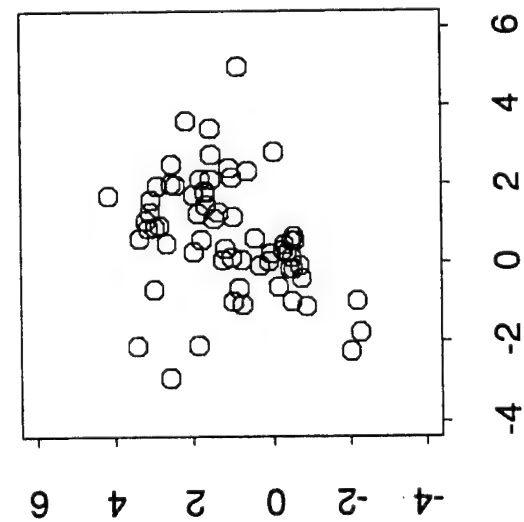
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(a) Unlabeled data

(b) Labeled data (o=component 1, +=component 2, and •=outlier data)

(c) Labeled data long with coutours of mixture population

(d) Contours of component populations and of outlier population (dotted)

Figure 1 - Mixture distributions for Example 2a where $f(x) = 5.N(\mu_1, \Sigma_1) + .5N(\mu_2, \Sigma_2)$
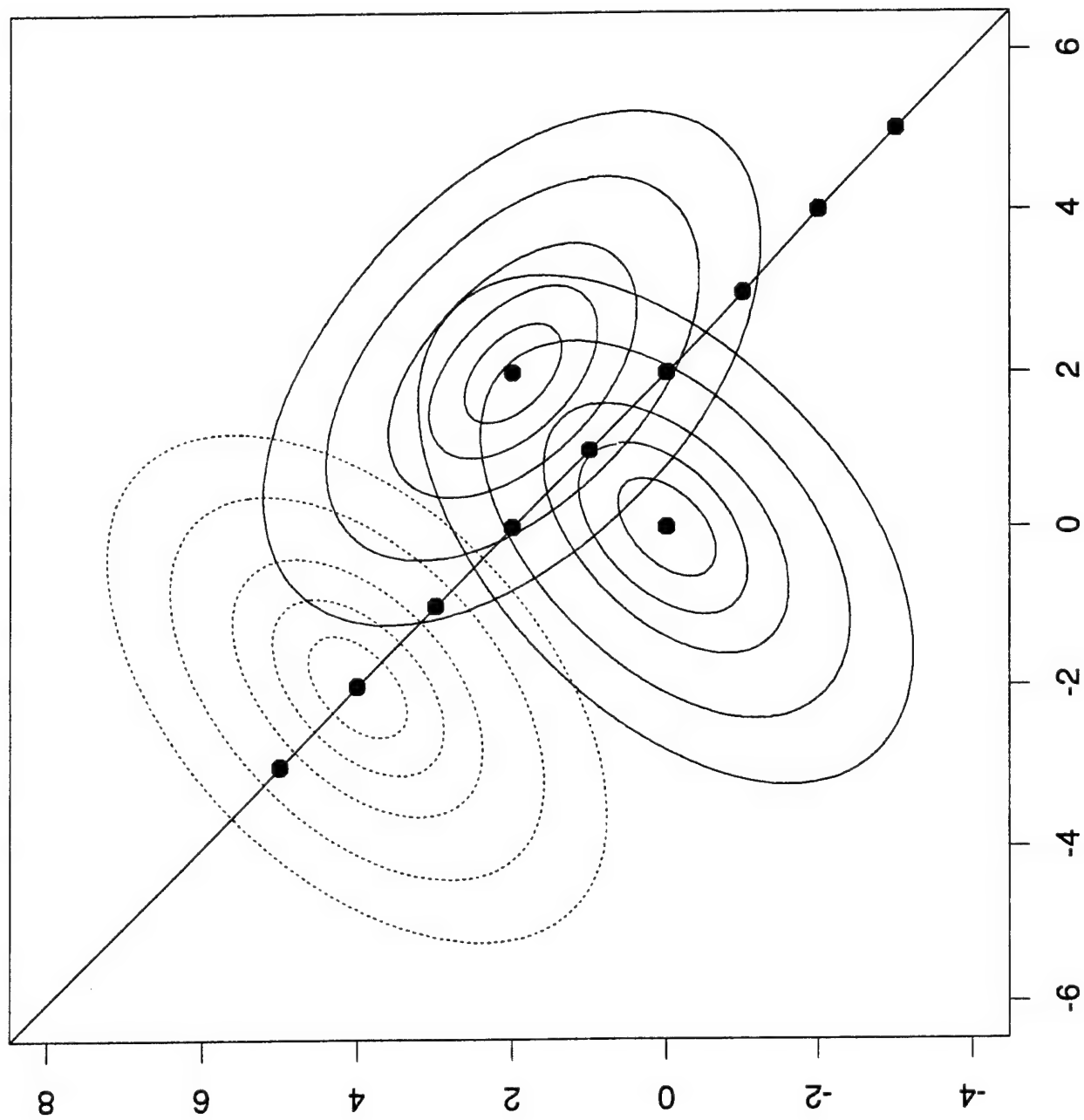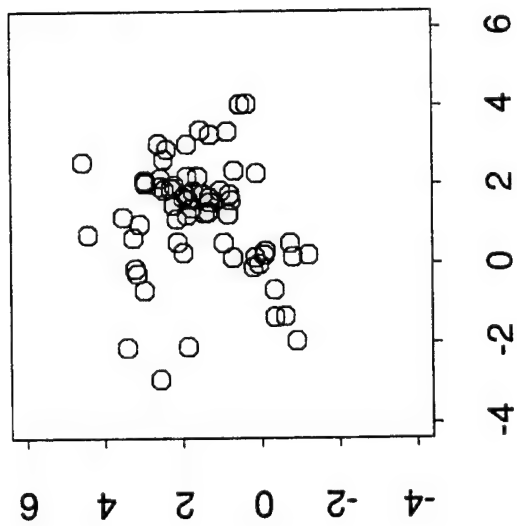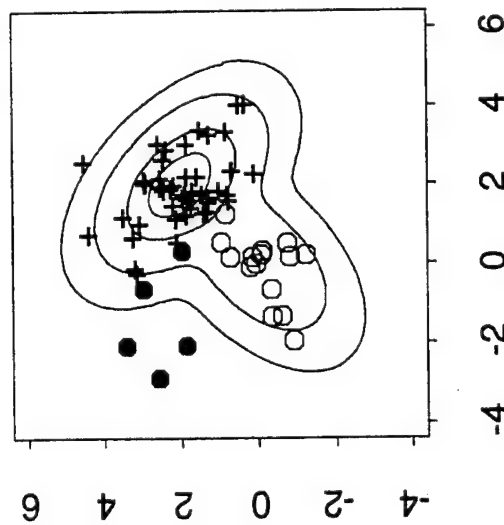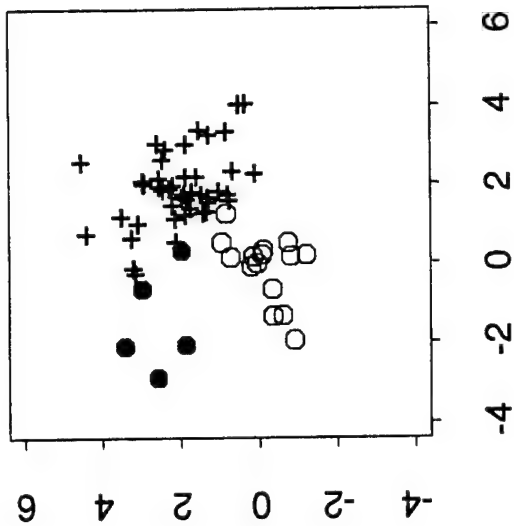
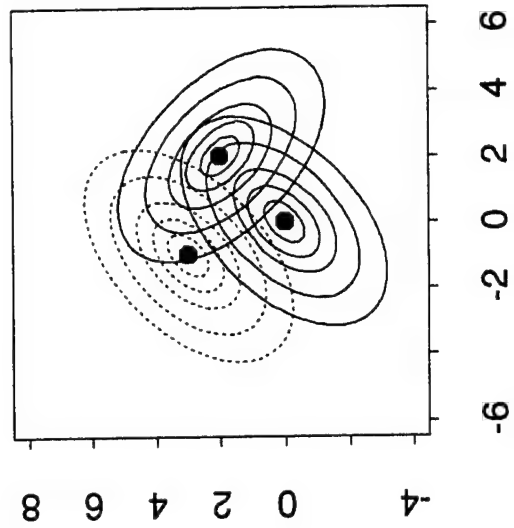Figure 2 - Mixture distributions for Example 2*a* showing means of outlier distributions in the simulations
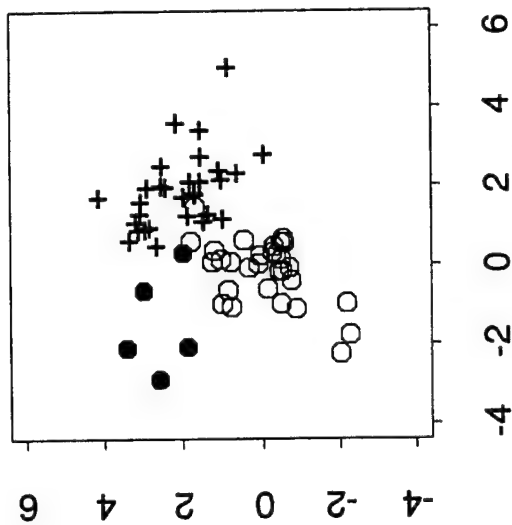
(a) Unlabeled data

(b) Labeled data (o=component 1, + =component 2, and ●=outlier data)
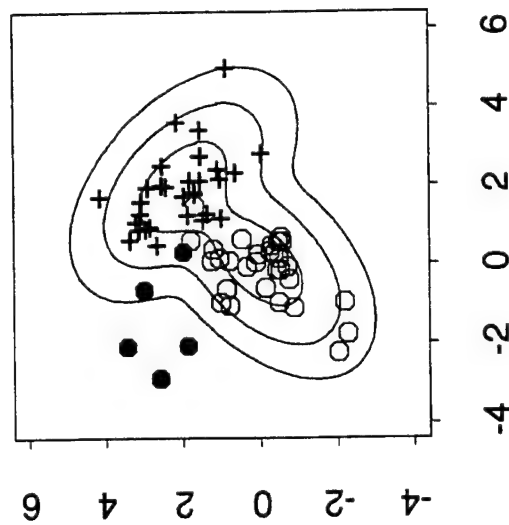
(c) Labeled data long with contours of mixture population

(d) Contours of component populations and of outlier population (dotted)

Figure 3 - Mixture distributions for Example 2b where $f(x) = .25N(\mu_1, \Sigma_1) + .75N(\mu_2, \Sigma_2)$

## 3.0    Positive Orthant Alternatives

In previous applications of outlier tests a symmetric alternative region has been assumed. This is, in general, not the best approach; and, it will clearly sacrifice power, i.e., reduce the detection probability. Since in most cases some information is known regarding the direction of the selected features relative to a nuclear event, an alternative region can be defined which takes advantage of this information. The resulting test would then be significantly more powerful. In this section we introduce some methodology for addressing this difficult problem.

## 3.1    Background

Since it is quite possible that a nuclear event is likely to occur in a region where no previous nuclear activity has transpired, a primary concern is to detect an unusual event. Let the $p$-dimensional variable $\mathbf{V} = (V_1, V_2, \ldots, V_p)$ characterize the occurrence of an event. The $V_i$ will be referred to as "script" variables or "features." Suppose that a training sample $\{\mathbf{V}_i\}_{i=1}^n$ is available from past events and a new observation, $\mathbf{V}_{n+1}$, is obtained which must be classified as to whether or not it belongs to the same population as the training sample. Baek, et. al. (1992) constructed a test for this situation by applying the parametric bootstrap (Efron (1979)) to generalized likelihood ratios. This approach, the bootstrapped generalized likelihood ratio test (BGLRT), was shown to be applicable when the observations are from either mixtures of discrete and normally distributed continuous variables or from a multivariate normal distribution. Miller, et. al. (1993) also showed that the BGLRT is also of utility when data are missing.

In the case where the observations are from a $p$-dimensional normal population, the likelihood ratio test leads to the two-sample Hotelling $T^2$ statistic and an $F$ statistic with $p$ and $n - p$ degrees of freedom. Bootstrapping this statistic amounts to empirically determining the critical points of the distribution of the statistic under the null hypothesis that the observation to be classified is a member of the population of interest. Through Monte Carlo investigation, the performance of the $T^2$ and the bootstrapped (either parametric or nonparametric) $T^2$ can be found to be effectively equivalent. Also at least in the one dimensional case, where exact tests are available for comparison, the nonparametric bootstrapped $T^2$ can be found to be quite robust to the effects of non-normality and to have reasonable power when compared to the appropriate uniformly most powerful test.

This report will examine the case where the observations are from a p-dimensional normal distribution. In this context, the $T^2$ statistic is testing the null hypothesis

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that the mean of the population associated with the training sample is equal to the mean of the population associated with the new observation versus the alternative that at least one of the elements of the mean is different.

In the situation of monitoring nuclear proliferation, it is possible that at least the order relationships of the individual features of the two populations may be known *a priori*. For example, if the observations were from a single monitoring station and were three dimensional, consisting of the frequency and the magnitude of the real and complex poles of an AR(3) model, then through analysis of existing data it is known that the complex pole of an explosion has a larger magnitude than the complex pole of an earthquake. Further, the frequency of the complex pole for an explosion will be less than that of an earthquake. Thus in testing the hypothesis that a given event is an earthquake versus the alternative hypothesis that it is an explosion, one would want the alternative region focused on large poles and small frequencies rather than simply "extreme poles" and "extreme frequencies." Such a region is called a "focused" alternative region.

It is desirable to take advantage of this before-hand knowledge by developing a test of hypothesis which is more focused than the standard two-sample $T^2$. Perlman (1969) developed theory for a single-sample $T^2$ with a one-sided alternative. In the single-sample problem, the null hypothesis of the standard $T^2$ is that the mean of a set of random observations is equal to zero versus the alternative that at least one of the elements of the mean is not equal to zero. His work was taken by Tang (1994) and applied to the alternative hypothesis that the sum of the elements of the mean is non-negative, a so-called half space alternative.

This report will expand the single-sample $T^2$ with one-sided alternative to the situation where the alternative hypothesis is that each element of the mean is positive. These results will then be extended to the special two-sample $T^2$ situation of interest in monitoring nuclear proliferation, in which the second sample consists of a single observation. Some Monte Carlo results will then be presented to illustrate the gains in power that can be achieved as contrasted with the standard two-sample $T^2$. No real data will be processed for this report. However, examples using real data will be included in the next report.

### 3.2    The Single-sample $T^2$ with a Half Space Alternative

A *half space* is a set of the form $\{v \mid v'u \geq 0\}$ for some fixed vector **u**. A set is *one-sided* if it is contained in the interior of a half space. A *cone* means a positively homogeneous, closed, and one-sided set. For the one-sample situation,

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it is assumed that there is a sample of size $n$ from a $p$-dimensional normal with unknown mean $\mu$ and covariance $\Sigma$. The problem is to test the null hypothesis that $\mu = 0$ versus the alternative hypothesis that $\mu \in C$, where $C$ denotes a cone.

Perlman derived the likelihood ratio statistic to be

$$U(\mathbf{x},\mathbf{y},A,C) = \|\mathbf{y}\|_A^2 (1 + \|\mathbf{y} - \mathbf{x}\|_A^2)^{-1}, \tag{1}$$

where $\mathbf{x}$ denotes $n^{\frac{1}{2}}$ times the sample mean, $A$ is $(n - 1)$ times the sample covariance matrix, and $\mathbf{y}$ is the vector in $C$ which is closest to $\mathbf{x}$ in terms of the Mahalanobis distance:

$$\|\mathbf{y} - \mathbf{x}\|_A^2 = (\mathbf{x} - \mathbf{y})' A^{-1}(\mathbf{x} - \mathbf{y}). \tag{2}$$

Tang proved that if $C$ contains an open set, and if $H^+$ is any half space containing $C$, then the test using the statistic $U(\mathbf{x},\mathbf{y},A,H^+)$ is uniformly more powerful than the statistic $U(\mathbf{x},\mathbf{y},A,C)$. He used a result of Perlman to calculate critical points for the statistic $U(\mathbf{x},\mathbf{y},A,H^+)$ and compared, via Monte Carlo results, the power of $U(\mathbf{x},\mathbf{y},A,H^+)$ versus the standard $T^2$.

## 3.3  Extension to the Positive Orthant Alternative Hypothesis

It is not possible to analytically calculate critical points for the test statistic $U(\mathbf{x},\mathbf{y},A,Q^+)$ in which $C$ is the positive orthant, $Q^+$, where all the elements of the mean are non-negative. However, bootstrapping provides a means of estimating the critical points of the statistic under the null hypothesis that the mean is zero. The process for conducting a test of size $\alpha$ using nonparametric bootstrapping is described in the following steps.

Procedure for the Bootstrap Test of the Null Hypothesis that the Mean of a Sample is Zero Versus the Alternative that the Mean is in the Positive Orthant

1. Compute the $U(\mathbf{x},\mathbf{m},A,Q^+)$ statistic using the original set of observations.

2. Subtract the mean of the sample from each of the observations, leaving the $n$ residuals.

3. Draw with replacement a random sample of size $n$ from the residuals (for which the null hypothesis holds conditionally).

4. For that sample, compute the statistic $U(\mathbf{x^*}, \mathbf{m^*}, A^*, Q^+)$, where the $*$ denotes the same quantities in (1) evaluated on the (re)sampled residuals.

5. Repeat steps 3 and 4 a total of $B$ times and save the values of $U^*$.

6. Calculate the $(1 - \alpha)$th quantile of these $B$ realizations, $u_{1-\alpha}$, the bootstrap estimate of the critical value.

7. If the statistic of step 1 equals or exceeds $u_{1-\alpha}$, the null hypothesis is rejected in favor of the alternative that $\mu \in Q^+$.

The main difficulty with carrying out the preceding steps is in the calculation of the statistic given by (1). If all the elements of the vector $\mathbf{x}$ are non-negative, then $\mathbf{y} = \mathbf{x}$, the denominator of (1) is unity, and the calculation involved is the same as that associated with the standard $T^2$ statistic. If, however, some or all of the elements of $\mathbf{x}$ are negative, then it remains to find the vector $\mathbf{y}$ in $Q^+$ which is closest to $\mathbf{x}$ in terms of the Mahalanobis distance. To develop a "feel" for the process the methodology for the two dimensional case will first be described and then a general procedure will be stated and summarized in a series of steps.

### 3.3.1 Calculation of $U(\mathbf{x}, \mathbf{y}, A, Q^+)$ in Two Dimensions

In the case where $p = 2$, let the $\mu_1$ axis be the abscissa and the $\mu_2$ axis be the ordinate. The positive quadrant, where values of $\mu_1$ and $\mu_2$ are positive, is labeled as quadrant 1. Quadrants 2 - 4 are found by moving counter-clockwise. So, if the first element of $\mathbf{x}$ is positive and the second element is negative, then $\mathbf{x}$ is located in quadrant 4, below the positive $\mu_1$ axis. This situation is depicted in Figure 1, which shows $\mathbf{x}$ at the center of an ellipse which is touching the $\mu_1$ axis at the point $\mathbf{y}_1 = (y_1, 0)$. The shape of the ellipse is governed by the elements of $A^{-1}$. The vector $\mathbf{y}_1$ is the closest point to $\mathbf{x}$ on the $\mu_1$ axis. It is the point which minimizes the distance:

$$q(\mathbf{y}_1) = (\mathbf{x} - (y_1, 0)')'A^{-1}(\mathbf{x} - (y_1, 0)'). \tag{3}$$

If the elements of the $A^{-1}$ matrix are denoted by $c_{ij}$, $i, j = 1, 2$, then the value of $y_1$ which minimizes (3) can be found to be:

$$y_1 = (c_{12}x_2 + c_{11}x_1)/c_{11}. \tag{4}$$

In the figure, $(y_1,0)$ is located on the non-negative part of the $\mu_1$ axis, and thus is a candidate to be the closest point in $Q^+$ to $\mathbf{x}$. In general, if $y_1$ were found to be negative, then the point $(0,0)$ would be the point in $Q^+$ closest to $\mathbf{x}$ and on the $\mu_1$ axis. There is also a point $\mathbf{y}_2 = (0,y_2)$ which is the closest point to $\mathbf{x}$ on the $\mu_2$ axis. It is the point which minimizes the distance:

$$q(\mathbf{y}_2) = (\mathbf{x} - (0,y_2)')'A^{-1}(\mathbf{x} - (0,y_2)'), \tag{5}$$

and the value of $y_2$ which minimizes (5) is:

$$y_2 = (c_{12}x_1 + c_{22}x_2)/c_{22}. \tag{6}$$

If $y_2$ were found to be negative (which it would be in Figure 1), then the point $(0,0)$ would be the point in $Q^+$ closest to $\mathbf{x}$ and on the $\mu_2$ axis. The value of $\mathbf{y}$ that is used in (1) is the one associated with the smaller of $q(\mathbf{y}_1)$ and $q(\mathbf{y}_2)$; otherwise, $\mathbf{y} = \mathbf{0}$, if neither $\mathbf{y}_1$ or $\mathbf{y}_2$ are in $Q^+$.

In summary, if $\mathbf{x}$ does not fall in the first quadrant, then depending on the quadrant in which it does fall and its sample covariance structure, there may or may not be a point $\mathbf{y}$ on the border of $Q^+$ other than the point $(0,0)$, in which case $U(\mathbf{x},\mathbf{y},A,Q^+)$ is equal to zero. The algorithmic approach for calculating the statistic $U(\mathbf{x},\mathbf{y},A,Q^+)$ in two dimensions is summarized in the following steps:

<u>Algorithm for Calculating $U(\mathbf{x},\mathbf{y},A,Q^+)$ in Two Dimensions</u>

1. Set $\mathbf{y} = \mathbf{0}$ and $d_{min} = \|\mathbf{x}\|_A^2$.

2. Using (4), calculate $y_1$. If $y_1 < 0$, go to step 4.

3. Calculate $q(\mathbf{y}_1)$ using (3). Set $\mathbf{y} = (y_1,0)'$ and $d_{min} = q(\mathbf{y}_1)$.

4. Using (6), calculate $y_2$. If $y_2 < 0$, go to step 6.

5. Calculate $q(\mathbf{y}_2)$ using (5). If $q(\mathbf{y}_2) < d_{min}$, set $\mathbf{y} = (0,y_2)'$.

6. The current value of $\mathbf{y}$ is used to calculate $U(\mathbf{x},\mathbf{y},A,Q^+)$ using (1).

### 3.3.2 Calculation of $U(x,y,A,Q^+)$ in $p$-Space

In $p$-space, the process of calculating the statistic $U(x,y,A,Q^+)$ is a generalization (albeit more complicated), of what is done in the case where $p = 2$. Again, if $\mathbf{x}$ is in the positive orthant $Q^+$, then $\mathbf{y} = \mathbf{x}$ and $U(x,y,A,Q^+)$ is equal to the standard $T^2$ statistic. Otherwise, the process is to find one or more points located on the periphery of $Q^+$, in the highest possible dimensional subspace, which are candidates in the positive orthant, and then determine which of those points is closest to $\mathbf{x}$. This is accomplished by initially searching in $(p - 1)$ space, then $(p - 2)$ space, and so forth, until either a point is found or else it is determined that there is no positive point on any of the p axes which is closest to $\mathbf{x}$.

Denote by $\mathbf{y}_{(j)}$ a vector with the $j$th element being zero, i.e., $\mathbf{y}_{(j)} = (y_1, y_2, ..., y_{j-1}, 0, y_{j+1}, ..., y_p)'$. The values of the elements of $\mathbf{y}_{(j)}$ are those which minimize the distance in the following equation:

$$q(\mathbf{y}_{(j)}) = (\mathbf{x} - \mathbf{y}_{(j)})'A^{-1}(\mathbf{x} - \mathbf{y}_{(j)}). \tag{7}$$

The elements of each $\mathbf{y}_{(j)}$ are obtained in the following manner. As before the elements of $A^{-1}$ are denoted by $c_{ij}$, $i,j = 1,2,...,p$, and set

$$\mathbf{d} = A^{-1}\mathbf{x}. \tag{8}$$

Let $C_{(j)}$ denote the $(p - 1) \times (p - 1)$ matrix obtained by deleting the $j$th row and column of $A^{-1}$, and designate by $\mathbf{d}_{(j)}$ the $(p - 1)$ vector realized when the $j$th element of $\mathbf{d}$ is deleted. The elements $y_1, y_2, ..., y_{j-1}, y_{j+1}, ..., y_p$ are found, respectively, as the $(p - 1)$ elements of the vector

$$\mathbf{z}_{(j)} = C_{(j)}^{-1} \mathbf{d}_{(j)}. \tag{9}$$

If any of the elements of $\mathbf{z}_{(j)}$ are negative, then the corresponding point $\mathbf{y}_{(j)}$ is not in the positive orthant. If there is more than one $\mathbf{y}_{(j)}$ in $Q^+$, then it can be determined which is the closest to $\mathbf{x}$.

If there is no $\mathbf{z}_{(j)}$ in which all of the elements are non-negative, then the search moves to the next lower dimension. This involves defining quantities $\mathbf{y}_{(i,j)}$, $C_{(i,j)}$,

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and $\mathbf{d}_{(i,j)}$, where, for example, $C_{(i,j)}$ is formed by deleting the $i$th and $j$th rows and columns of $A^{-1}$. Then one obtains $\mathbf{z}_{(i,j)}$ :

$$\mathbf{z}_{(i,j)} = C_{(i,j)}^{-1} \mathbf{d}_{(i,j)}. \tag{10}$$

There are $\binom{p}{p-2}$ possibilities to examine before moving to the next lower dimension, if required. Each time the dimensionality decreases, the number of elements of $\mathbf{d}$ which are used decreases by one, and one more row and column of $A^{-1}$ are not used. Eventually, if there is no point in $Q^+$ which is found to be closest to $\mathbf{x}$, then $\mathbf{y} = \mathbf{0}$ and $U = 0$. This situation would require the maximum of $2^p - 1$ searches for $\mathbf{y}$.

## 3.4 Application to a Training Sample and Classification of a New Observation

The extension of the single-sample test of hypothesis, that the mean is zero versus the focused alternative that the mean is in the positive orthant, to the case of interest in this report, requires minor modifications to the procedure outlined in the single-sample case. Let the $p$-dimensional variable $\mathbf{V} = (V_1, V_2, \ldots, V_p)$ characterize the occurrence of an event. Suppose that a training sample $\{\mathbf{V}_i\}_{i=1}^{n}$ is available from past events and a new observation, $\mathbf{V}_{n+1}$, is obtained which must be classified as to whether or not it belongs to the same population as the training sample. Denote by $\bar{\mathbf{V}}$ the mean of the training sample observations and let $\mathbf{x} = \mathbf{V}_{n+1} - \bar{\mathbf{V}}$. The counterpart to (1) for the test statistic for this special two-sample case is:

$$U(\mathbf{x}, \mathbf{y}, A, Q^+) = \|\mathbf{y}\|_A^2 \left((n+1)/n + \|\mathbf{y} - \mathbf{x}\|_A^2\right)^{-1}, \tag{11}$$

where, as before, $\mathbf{y}$ is the closest point in $Q^+$ to $\mathbf{x}$ as measured by (2). Other than the different definition of $\mathbf{x}$ and using (11) in lieu of (1), the only other difference is that it is necessary to add a step in the bootstrapping test procedure in which a single observation is drawn in addition to the training set. With regards to finding the closest vector to $\mathbf{x}$, all the equations and procedures of the previous sections are applicable. The process to conduct the desired test of hypothesis of size $\alpha$ is summarized in the following steps.

Procedure to Test the Null Hypothesis that the Mean of a New Observation is Equal to the Mean of a Training Sample Versus the Alternative that the Mean of the New Observation is in the Positive Orthant

1. Compute $U(\mathbf{x}, \mathbf{y}, A, Q^+)$ using the original set of observations and (11)

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2. Subtract the mean of the training sample from each of the observations in the training sample, leaving the $n$ residuals

3. Obtain a bootstrapped training sample by drawing with replacement a random sample of size $n$ from the residuals

4. Obtain a bootstrapped new observation by drawing one of the residuals with replacement

5. For those samples, compute the statistic $U(\mathbf{x}^*, \mathbf{y}^*, A^*, Q^+)$, where the * denotes the same quantities in (11) evaluated on the (re)sampled residuals

6. Repeat steps 3 to 5 a total of $B$ times and save the values of $U^*$

7. Calculate the $(1 - \alpha)$th quantile of the $B$ realizations, $u_{1-\alpha}$, the bootstrap estimate of the critical value

8. If the statistic of step 1 equals or exceeds $u_{1-\alpha}$, the null hypothesis is rejected in favor of the alternative

To illustrate the improved power that is realized with the focused alternative hypothesis, a sequence of Monte Carlo experiments was conducted in which the standard $T^2$ was contrasted to the focused alternative. In two dimensions, observations in a training sample were randomly generated with parameters:

$$\mu_1 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ and } \Sigma_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},$$

while the observation $\mathbf{V}_{n+1}$ was randomly generated with the same covariance matrix and a mean:

$$\mu_2 = \begin{pmatrix} \Delta \\ \Delta \end{pmatrix}.$$

Power was based on 1,000 replications at each value of $\Delta$. It was estimated based on the proportion of the 1,000 iterations in which $\mathbf{V}_{n+1}$ was found to be in the critical region. The value of $B$, the number of bootstraps used in obtaining a focused alternative critical point, was selected to be 499. The desired significance level for the test was $\alpha = 0.05$. Figure 2 presents the results for a training sample of 30. An interesting feature of this figure is that the test based on the statistic $U(\mathbf{x}, \mathbf{y}, A, Q^+)$ has virtually no power for negative values of $\Delta$ while displaying

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considerably more power than the standard two-sample $T^2$ when $\Delta$ is in the first quadrant.

When the number of dimensions is increased to four, the improvement of $U(\mathbf{x},\mathbf{y},A,Q^+)$ over the $T^2$ is even more impressive, as illustrated in Figure 3. To obtain this figure, the numbers of bootstraps and replications remained the same as with $p = 2$, while the statistical distribution parameters were:

$$\mu_1 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \mu_2 = \begin{pmatrix} \Delta \\ \Delta \\ \Delta \\ \Delta \end{pmatrix}, \text{ and } \Sigma_1 = \Sigma_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

## 3.5    Conclusion

In monitoring nuclear proliferation, it is possible that at least the relative order relationships of the individual features of two different populations may be known *a priori*. In this report a test of hypothesis employing a focused alternative region, for taking advantage of such a situation in classifying new observations, is described. The methodology to employ when using this test is outlined; and, representative results for different sample sizes and feature dimensions are presented. These results indicate that this test should be a useful tool in the classification process.

## 3.6    References

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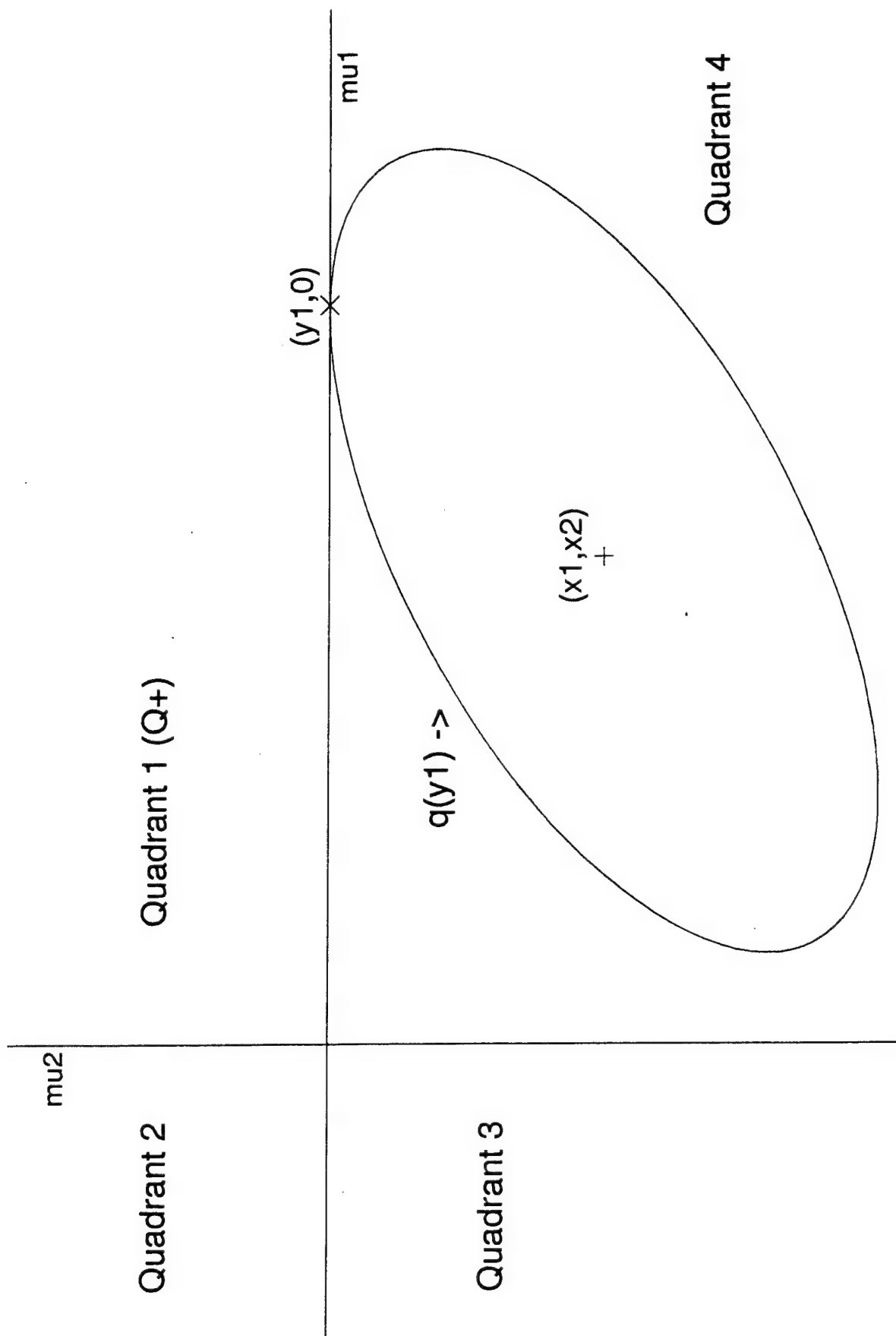
Figure 1: Closest Point in Q+ to Point in Quadrant 4
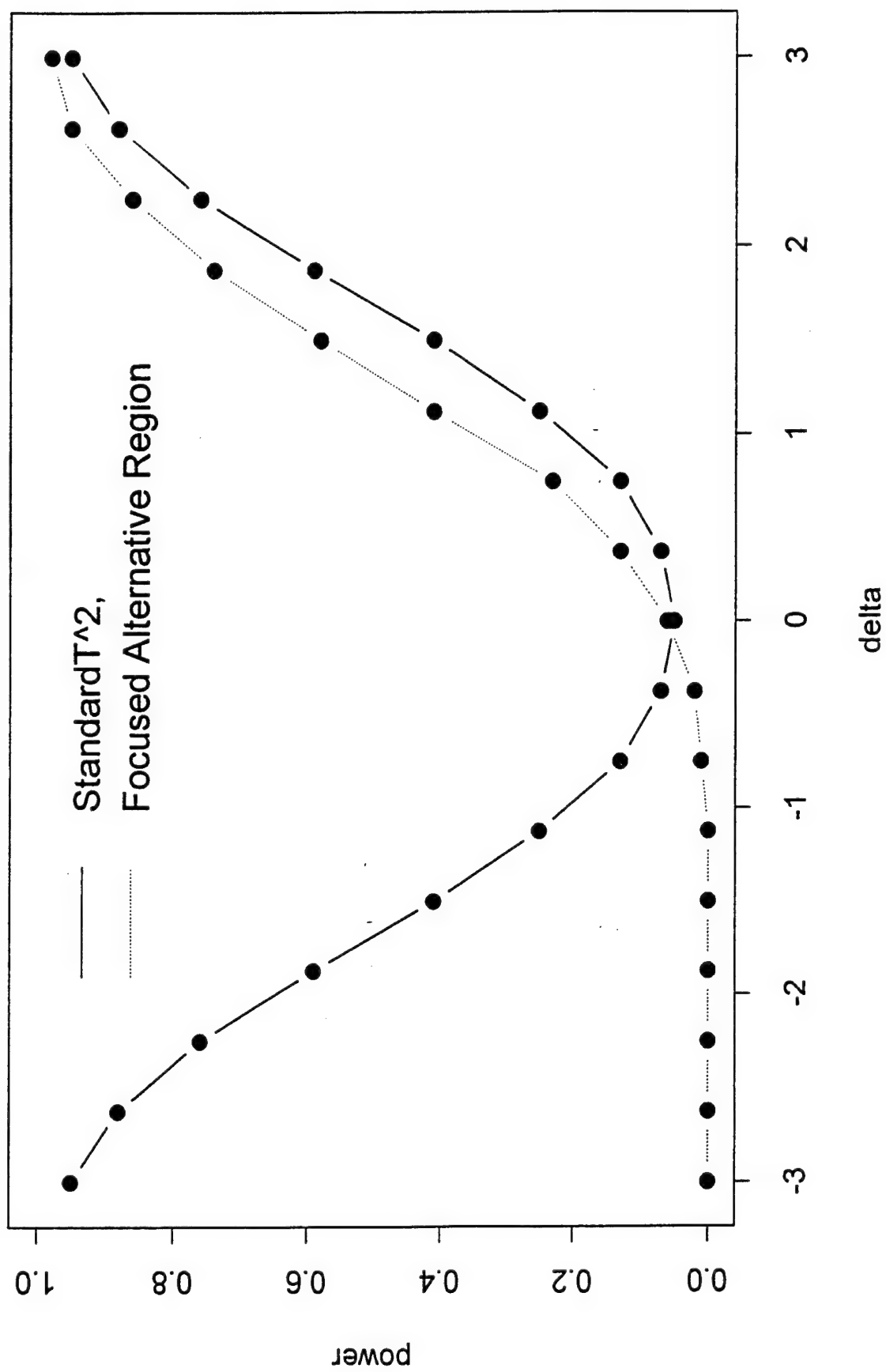
Figure 2: Power Comparison for Two Dimensions (n=30)
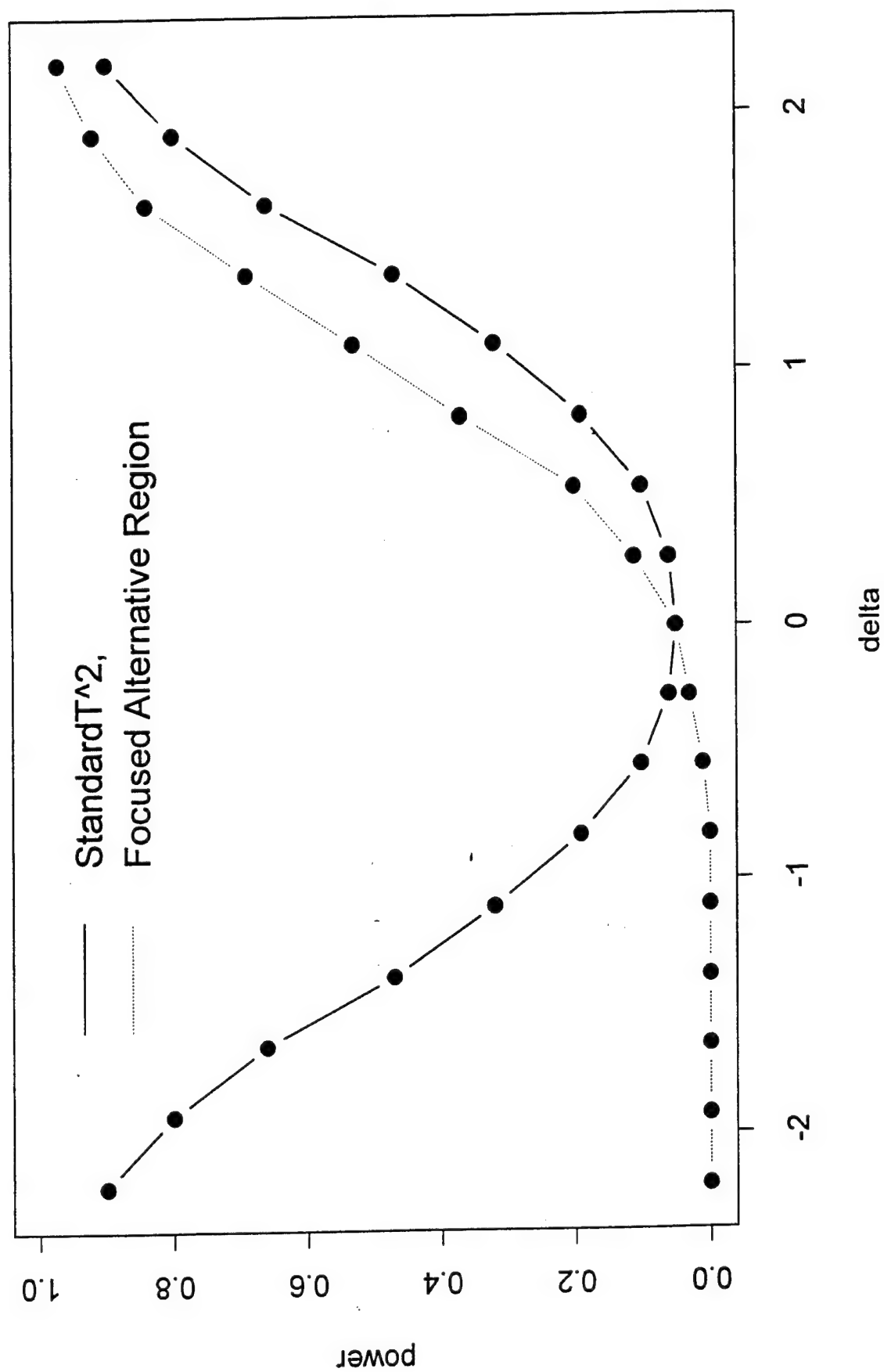
Figure 3: Power Comparison for Four Dimensions (n=30)

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